A 3-D Extension of the Multiscale Control Volume Method for the Simulation of the Steady-State Diffusion Equation

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Abstract. The level of detail on modern geological models requires higher resolution grids that may render the simulation of multiphase flow in porous media intractable. Moreover, these models may comprise highly heterogeneous media with phenomena taking place in different scales. The Multiscale Finite Volume (MsFV) method can tackle such issues by constructing a set of numerical operators that map quantities from the fine-scale domain to a coarser one where the initial problem can be solved at a lower computational cost and the solution mapped back to the original scale. Unlike more traditional techniques like homogenization and upscaling, the MsFV has the advantage of maintaining the coupling between the scales even when there is no clear scale separation. However, the MsFV formulation is limited to k-orthogonal grids since it uses a Two-point Flux Approximation (TPFA) method and employs an algorithm to generate the coarse meshes that is not capable of handling general geometries. The Multiscale Restriction Smoothed-Basis method (MsRSB) improves on the MsFV by introducing a new iterative procedure to find the multiscale operators and modifying the algorithm for the generation of the multiscale geometric entities to accommodate unstructured coarse grids, but is still limited to structured fine grids due to the TPFA discretization. Finally, the Multiscale Control Volume method (MsCV) replaces the TPFA by the Multipoint Flux Approximation with a Diamond stencil (MPFA-D) scheme on the fine-scale while further enhancing the generation of the geometric entities to allow truly unstructured grids on the fine and coarse scales for two-dimensional simulation. In this work we propose an extension to three-dimensional geometries of both the MsCV and the algorithm to obtain the multiscale geometric entities based on the concept of background grid. We also modify the MPFA-D to use the very robust Generalised Least Squares (GLS) interpolation technique to obtain the required auxiliary nodal unknowns. We show that the 3-D MsCV method produces satisfactory results even for heterogeneous and highly anisotropic media, employing true unstructured grids on both scales to handle the simulation of the steady-state diffusion equation.

Keywords: MsCV, MPFA-D, GLS, background grid, steady-state diffusion problem

1 Introduction

The numerical simulation of physical phenomena is a fundamental step to verify and predict how a proposed model will behave in a real world scenario. In the context of the Finite Volume formulations, this may involve discrete models whose resolution ranges from 10^8 to 10^9, as pointed out by Jaramillo et al. [1]. Moreover, the study can comprise phenomena happening in different scales and highly heterogeneous media, as it is often the case for the flow simulation in porous media, discussed by Hajibeygi et al. [2]. For this purpose, scale transferring techniques are employed. Upscaling techniques can be used to obtain an approximate solution on a lower resolution grid, as seen in Farmer [3], but may induce to loss of physical characterization. On the other hand, multiscale methods can keep the coupling between scales through numerical operators.

We turn our attention to the Multiscale Finite Volume (MsFV) family of methods, originally proposed by Jenny et al. [4]. Within this family of methods, we highlight the Multiscale Restriction-Smoothed Basis (MsRSB) by Møyner and Lie [5], who introduce an iterative formulation for the multiscale operators, and the Multiscale Control Volume (MsCV) by de Souza et al. [6] which improves on the MsRSB by enabling the use of unstructured grids on all scales for 2-D models. This is done by using a consistent fine-scale flux approximation in the form of the Multipoint Flux Approximation with a Diamond stencil from Contreras et al. [7], and modifying the multiscale pre-processing algorithm.

In this work, we propose an extension of the MsCV to 3-D geometries coupled with the 3-D MPFA-D from de Lira Filho et al. [8] and the robust GLS interpolation introduced by Dong and Kang [9]. In order to generate the multiscale geometric entities, we also extend the background grid framework proposed by de Souza et al. [10] to 3-D geometries. Finally, we introduce an enhanced version of the 3-D MsCV, the E-MsCV, by incorporating the preconditioning technique from the E-MsRSB by Bosma et al. [11] to the definition of the multiscale operators.

2 Mathematical formulation

The 3-D steady-state diffusion equation in anistropic and heterogeneous media is given by:

$$\nabla \cdot \overrightarrow{\mathcal{F}} = \mathcal{Q}(\overrightarrow{x}), \text{with } \overrightarrow{\mathcal{F}} = -\underset{\sim}{\mathcal{K}}(\overrightarrow{x})\nabla u \text{ for } \overrightarrow{x} \in \Omega \subset \mathbb{R}^3, \tag{1}$$

where $\overrightarrow{\mathcal{F}}$ is a diffusive flux, u is a scalar field, $\underset{\sim}{\mathcal{K}}(\overrightarrow{x})$ is a diffusion tensor, and $\mathcal{Q}(\overrightarrow{x})$ is the source term.

Typical boundary conditions for eq. (1) are:

$$u = g_D \quad \text{for } \overrightarrow{x} \in \Gamma_D, \tag{2}$$

$$\overrightarrow{\mathcal{F}}(\overrightarrow{x}) \cdot \overrightarrow{n} = g_N \quad \text{for } \overrightarrow{x} \in \Gamma_N, \tag{3}$$

where $\partial\Omega = \Gamma_D \cup \Gamma_N$, Γ_D and Γ_N represent the Dirichlet and Neumann boundaries, respectively, such that $\Gamma_D \cap \Gamma_N = \varnothing$, and $\overrightarrow{n}$ is the unit outward normal vector.

3 Numerical formulation

Equation (1) is discretized using the Multipoint Flux Approximation with a Diamond stencil (MPFA-D) by de Lira Filho et al. [8], a full pressure support Finite Volume scheme for 3-D tetrahedral meshes. Given the arrangement shown in Fig. 1, the flux through the internal face IJK is approximated by:

$$\overrightarrow{\mathcal{F}}_{\hat{R}} \cdot \overrightarrow{N}_{IJK} \approx -K^n_{eff}\left[2(u_{\hat{R}} - u_{\hat{L}}) - D_{JI}(u_I - u_J) - D_{JK}(u_K - u_J)\right], \tag{4}$$

where $\overrightarrow{N}_{IJK}$ is a normal vector to the face IJK, K^n_{eff} is the face transmissibility, D_{JI} and D_{JK} are the cross diffusion terms, $u_{\hat{R}}$ and $u_{\hat{R}}$ are the cell centered unknowns, and u_I, u_J and u_K are vertex centered unknowns.

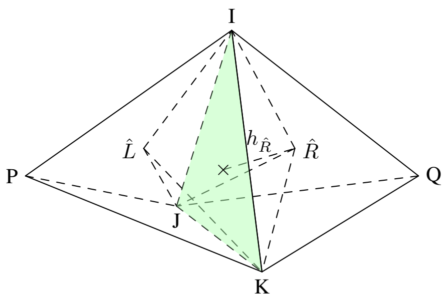


Figure 1. Two tetrahedra $\hat{R}$ and $\hat{L}$ sharing a face IJK illustrating the main entities in the MPFA-D scheme. Adapted from de Lira Filho et al. [8].

3.1 Boundary conditions

For faces on the Dirichlet boundary, the flux term is defined as:

$$\overrightarrow{\mathcal{F}}_{\hat{R}} \cdot \overrightarrow{N}_{IJK} \approx -\left[2\frac{K^n_{\hat{R}}}{h_{\hat{R}}}(u_{\hat{R}} - g^D_J) + D_{JI}(g^D_J - g^D_I) + D_{JK}(g^D_J - g^D_K)\right], \quad (5)$$

where g^D_I, g^D_J and g^D_K are the prescribed values on the boundary. On the Neumann boundary, the boundary conditions are given by:

$$\overrightarrow{\mathcal{F}}_{\hat{R}} \cdot \overrightarrow{N}_{IJK} = g_N. \quad (6)$$

For a more detailed explanation on the construction of the flux approximation, refer to de Lira Filho et al. [8].

3.2 Vertex unknowns interpolation

As it can be seen from Equation (4), the MPFA-D's unique flux expression, apart from the cell unknowns, includes vertex unknowns that must be eliminated in order to obtain a completely cell-centered approximation. This can be achieved by rewriting the vertex variables as a linear combination of the surrounding cell-centered values:

$$u_v = \sum_{\hat{k}=1}^{n_k} \omega_{\hat{k}} u_{\hat{k}}. \quad (7)$$

Here, we have opted to use the Global Least Squares (GLS) interpolation by Dong and Kang [9]. It is a linear-preserving interpolation technique capable of handling heterogeneous and highly anisotropic media while maintaining a good convergence rate as discussed by de Moura Cavalcante [12]. The weights in the GLS interpolation are computed via the solution in the least squares sense of a set of local problems for each node. For a more intricate discussion of the assembly and definition of the local problems to find the interpolation weights, refer to Dong and Kang [9].

4 The 3-D Multiscale Control Volume method

4.1 The MsCV framework

The Multiscale Control Volume (MsCV) method, as originally proposed by de Souza et al. [6] for 2-D models, is a multiscale formulation that constructs an approximation of the solution on the fine-scale via two operators: the prolongation operator $\mathbf{P}$ and the restriction operator $\mathbf{R}$. Let $\mathbf{u}$ and $\mathbf{u}_c$ denote the fine-scale and the coarse-scale solutions, respectively, and the fine-scale system of equations $\mathbf{Au} = \mathbf{q}$. The MsCV approximation is given by:

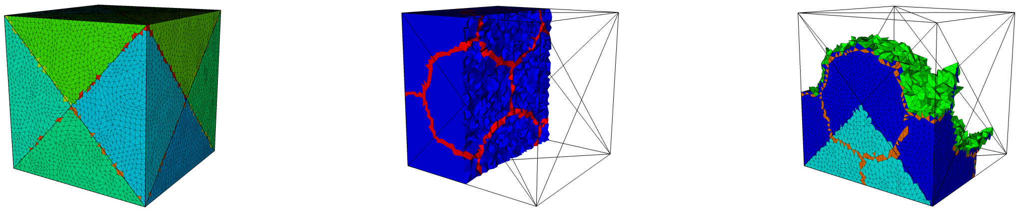
$$\mathbf{u} \approx \mathbf{u}_{ms} = \mathbf{P}\mathbf{u}_c. \quad (8)$$

The coarse-scale solution is found by solving the coarse-scale system of equations $\mathbf{A}_c\mathbf{u}_c = \mathbf{q}_c$ such that $\mathbf{A}_c = \mathbf{RAP}$ and $\mathbf{q}_c = \mathbf{Rq}$.

In order to properly define the MsCV operators, some geometric entities must be generated. Given the fine-scale grid Ω^f, first, the primal coarse grid (Ω^P_c) is formed by partitioning the fine-scale grid into coarse blocks. For this grid, centers are also defined as the fine-scale volumes whose centroids are the closest to the primal coarse volume's centroid. A dual coarse grid (Ω^D_c) is also generated as way to impose mass conservation on the coarse scale. Moreover, for each primal coarse volume, a support region is delimited as its region of influence, i.e., where its basis function is non-null. In the proposed framework, all these entities are generated using a background grid Ω^{bg}, concept first introduced in the multiscale context by de Souza et al. [10]. The aforementioned entities are illustrated in Fig. 2.

4.2 The MsCV operators in 3-D

The MsCV prolongation operator is computed through an iterative procedure based on the Multiscale Restriction Smoothed Basis (MsRSB) method proposed by Møyner and Lie [5]. The operator's basis functions are updated through a series of weighted Jacobi iterations of the form:



(a) The primal coarse grid Ω_c^P.

(b) The dual coarse grid Ω_c^D (red).

(c) An example of support region I_j (dark and light blue), its boundary B_j (green) and the intersection with other boundaries (orange).

Figure 2. Illustration of the MsCV geometric entities.

$$P_j^{n+1} = P_j^n - \varpi D^{-1} A^{pre} P_j^n. \tag{9}$$

where ϖ is the relaxation parameter of the Jacobi iteration set to $2/3$, D^{-1} is the inverse of the main diagonal of the preconditioned MPFA-D left-hand side term, and A^{pre} is the preconditioned MPFA-D matrix. Here, the preconditioned matrix is a direct application of the technique described by de Souza et al. [6] and is given by:

$$A_{ij}^{pre} = \begin{cases} A_{ij} & \text{if } i \neq j \\ A_{ii} - \sum_{k=1}^{n_f} A_{ik} & \text{otherwise} \end{cases}. \tag{10}$$

A more intricate discussion of iterative procedure can be found in de Souza et al. [6] and Alves et al. [13].

Finally, for the restriction operator, we use the Finite Volume restriction operator from Jenny et al. [4] defined as:

$$\mathbf{R}_{ij} = \begin{cases} 1 & \text{if } \Omega^{f,j} \in \Omega_{c,i}^P \\ 0 & \text{otherwise} \end{cases}. \tag{11}$$

4.3 The Enhanced MsCV (E-MsCV)

As discussed by [11], the MsRSB prolongation operator may show slow convergence when applied to non M-matrices. To overcome this issue, a modification to the fine-scale matrix is suggested so that the M-matrix properties are reinforced, making the convergence rate of the method closer to when it is applied to a TPFA matrix.

The 3-D MsCV presents the same convergence issues. Since the MsCV prolongation operator is based on the MsRSB, it is natural to consider the application of the aforementioned procedure to our new framework. We designate this modified version of the MsCV the *Enhanced MsCV* (E-MsCV). The preconditioning technique applied is defined as:

$$A_{ij}^{*} = \min\left(A_{ij}, 0\right) \text{ for } i \neq j, \tag{12}$$

$$A_{ij}^{pre} = \begin{cases} A_{ij}^{*} & \text{if } i \neq j \\ A_{ii}^{*} - \sum_{k=1}^{n_f} A_{ik}^{*} & \text{otherwise} \end{cases}. \tag{13}$$

5 Numerical results

In this section, we present an example to illustrate a simulation performed using both the 3-D MsCV and the E-MsCV. To compare the quality of the solutions, the following error norms were used:

$$||\mathbf{u}^{ref} - \mathbf{u}^{ms}||_2 = \left(\frac{\sum_{\Omega_i \in \Omega_f} |u_i^{ref} - u_i^{ms}|^2}{\sum_{\Omega_i \in \Omega_f} |u_i^{ref}|^2} \right)^{1/2}, \tag{14}$$

$$||\mathbf{u}^{ref} - \mathbf{u}^{ms}||_\infty = \frac{\max_{\Omega_i \in \Omega_f} |u_i^{ref} - u_i^{ms}|}{\max_{\Omega_i \in \Omega_f} |u_i^{ref}|}, \tag{15}$$

where the superscripts ms and *ref* correspond to the multiscale solution and the reference fine-scale solution, respectively.

We study the simulation of a single-phase flow in a reservoir with a spherical heterogeneity within the domain $\Omega = [-2, 2]^3$. The following boundary conditions are applied:

$$\begin{cases} g_D = 0 & \text{on } \Gamma_{D,1} \\ g_D = 1 & \text{on } \Gamma_{D,2} \\ g_N = 0 & \text{on } \Gamma_N \end{cases}, \tag{16}$$

where $\Gamma_{D,1}$ corresponds to the planes $x = -2$, $\Gamma_{D,2}$ corresponds to the plane $x = 2$, and Γ_N is set at the planes $y = -2$, $y = 2$, $z = -2$ and $z = 2$.

The heterogeneity region is shaped as a sphere centered at the origin with a radius equal to 0.75 embedded in a homogeneous domain with a permeability tensor given by:

$$\underset{\sim}{K}_1(x, y, z) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{17}$$

Two configurations were simulated, a barrier and a channel, with permeability tensors respectively given by:

$$\underset{\sim}{K}_2(x, y, z) = \begin{pmatrix} 10^{-3} & 0 & 0 \\ 0 & 10^{-3} & 0 \\ 0 & 0 & 10^{-3} \end{pmatrix}, \tag{18}$$

$$\underset{\sim}{K}_3(x, y, z) = \begin{pmatrix} 10^{3} & 0 & 0 \\ 0 & 10^{3} & 0 \\ 0 & 0 & 10^{3} \end{pmatrix}. \tag{19}$$

The simulations were conducted in a fine-scale grid with 159,893 tetrahedral cells and the multiscale grids were generated using a structured $6 \times 6 \times 6$ hexahedral background grid.

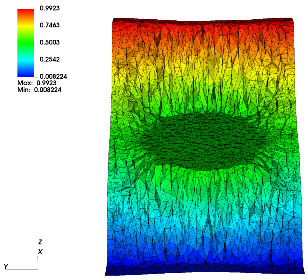
(a) Barrier configuration. (b) Channel configuration.

Figure 3. Fine-scale reference solutions for the single-phase simulation of a reservoir containing a spherical heterogeneity under a barrier (a) and channel (b) configuration. Slice at $y = 0$.

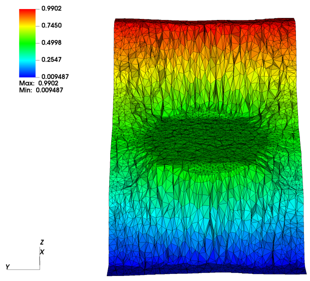
The multiscale solutions are presented in Fig. 4 for each MsCV formulation and each configuration. For the channel setup, the solutions remain qualitatively close to the fine-scale reference solution shown in Fig. 3b. The

Table 1. The L_2 and L_∞ norms of the errors for the simulation of a reservoir containing a spherical heterogeneity.

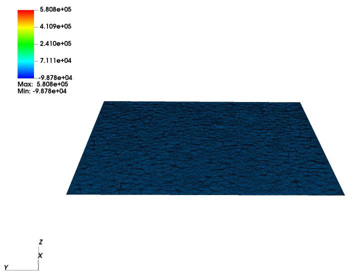
Error (%)	**Channel**		**Barrier**	
	MsCV	E-MsCV	MsCV	E-MsCV
$\|\|u\|\|_2$	0.69	0.59	7×10^8	6.02
$\|\|u\|\|_\infty$	18.79	19.04	5×10^7	83.78



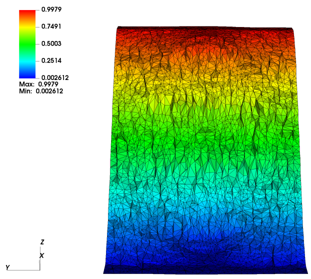
(a) Channel configuration, MsCV solution.



(b) Channel configuration, E-MsCV solution.



(c) Barrier configuration, MsCV solution.



(d) Barrier configuration, E-MsCV solution.

Figure 4. The multiscale solutions for different configurations for the spherical heterogeneity. Slice at $y = 0$.

errors in Table 1 corroborate with the observation, as the L_2 norm of the error is approximately 0.6% for both the 3-D extension of the MsCV and the E-MsCV despite considerable values for the L_∞ norm of the errors.

Regarding the iterative performance of the multiscale methods, the original MsCV's iterations present a slower convergence rate and did not converge on the prescribed tolerance criterion equal to 10^{-3}, requiring to stop the iterative procedure after 500 iterations to achieve a result with errors of the same magnitude as those presented by the E-MsCV, which in turn took 132 iterations.

In a barrier configuration, the solution using the original MsCV preconditioning fails to converge regardless of the background grid used. On the other hand, the E-MsCV converges. Albeit not able to fully capture the barrier in the reservoir, the E-MsCV's solution still manages to reasonably show its main features on both background grids and it is a good initial guess for a smoothing procedure. As seen in Table 1, the L_2 norm of the errors on the solution using the E-MsCV are still satisfactory even though the L_∞ norm of the error is very high.

6 Conclusions

In this work, we have proposed a 3-D extension and an enhance version of the MsCV method. From our experiments, the 3-D MsCV is capable of approximating the reference fine-scale solution to a good degree on low to intermediate complexity scenarios and the E-MsCV is able to converge on more challenging scenarios. It was also possible to notice that, despite of the robustness of the MPFA-D with the GLS interpolation, there are violations of the DMP which are exacerbated in the multiscale solution. In the near future, we intend to explore new approaches to generate the multiscale geometric entities under the background grid framework by adapting them to the underlying geological characteristics, to study smoothing techniques and to investigate algebraic multiscale strategies in place of the MsRSB. Furthermore, we also intend to address the DMP violation issue by introducing a defect correction scheme similar to the one proposed by [14, 15] and to expand the work to the simulation of multiphase flows in heterogeneous and anisotropic porous media.

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